

Modulation spectroscopy with ultracold fermions in an optical lattice

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We propose an experimental setup of ultracold fermions in an optical lattice to determine the pairing gap in a superfluid state and the spin ordering in a Mott-insulating state. The idea is to apply a periodic modulation of the lattice potential and to use the thereby induced double occupancy to probe the system. We show by full time-dependent calculation using the adaptive time dependent density-matrix renormalization group method that the position of the peak in the spectrum of the induced double occupancy gives the pairing energy in a superfluid and the interaction energy in a Mott-insulator, respectively. In the Mott-insulator we relate the spectral weight of the peak to the spin ordering at finite temperature using perturbative calculations.

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The use of Feshbach resonances [1] and the loading of ultracold atoms into optical lattices [2, 3] opened up the possibility to realize strong interactions in quantum gases. These systems provide outstanding control over most of their parameters, which offers the possibility to use them as ‘quantum simulators’ [4], i.e. to investigate unresolved questions from quantum many-body physics in a well-controllable system. One example is the crossover between a Bose-Einstein condensate of bosonic molecules and a BCS-like state of fermionic atoms [5, 6]. A major step in the direction to ‘simulate’ phenomena in periodic potentials has been taken by Köhl *et al.* [7] and very recently by Chin *et al.* [8] who succeeded in loading ultracold fermions into a three-dimensional optical lattice.

However, the possibilities to probe ultracold gases in optical lattices are still very limited as compared to measurement techniques in condensed matter systems. On top of this some of the known probes for bosonic gases are not useful in the context of fermionic gases. Thus the lately experimental realization demands for new techniques. We propose an experimental setup to measure the pairing energy of a superfluid state and the interaction strength in a Mott-insulating or liquid state of a two component mixture of fermionic atoms in an optical lattice. Proposals how to gain information about the pairing in a superfluid state have been made for example in Ref. [9, 10, 11] for a system without a lattice and in Ref. [12] with a lattice. The setup proposed here is based on the experiment by Stöferle *et al.* [13] in which a gas of ultracold bosons was probed using the energy absorption induced by periodic modulations of the lattice potential. It has been shown that very precise information about the excitation structure of a bosonic system [14, 15, 16, 17, 18, 19], and about the degree of incommensurate filling [19] can be extracted by means of this experiment. It would therefore be desirable to extend the measurement to fermionic systems. However, in a fermionic system the energy absorption cannot be determined in the same way as it was done in the bosonic setup. There the energy absorption imprints a clear characteristic signal in time-of-flight mea-

surements which is not the case for fermionic systems. In the present work we therefore propose to probe a two-component fermionic mixture by the observation of the double occupancy which is induced by a periodic modulation of the lattice potential. The double occupancy can be observed by projecting double occupied sites onto molecules [20]. We show that this measurement gives information on the pair binding energy of the superfluid state and the interaction energy in a liquid or Mott-insulating state. We further propose how information on the spin ordering could be extracted in the case of repulsive interaction.

In our studies we focus on a two component fermionic gas which is tightly confined to one dimensional tubes along the x -direction by a strong lattice in the transverse directions. Such a system was realized in the experiment [21]. If an additional periodic potential V_x is applied along the tubes, the system can be described [12, 22] by the Hubbard model

$$H = -J \sum_{j,\sigma} \left(c_{j,\sigma}^\dagger c_{j+1,\sigma} + h.c. \right) + U \sum_{j,\sigma} \hat{n}_{j,\uparrow} \hat{n}_{j,\downarrow}. \quad (1)$$

Here $\sigma = \{\uparrow, \downarrow\}$ labels the two hyperfine states, $c_{j,\sigma}^\dagger$ and $c_{j,\sigma}$ are the corresponding creation and annihilation operators, and $\hat{n}_{j,\sigma} = c_{j,\sigma}^\dagger c_{j,\sigma}$ is the number operator on site j . The values of hopping parameter J and the interaction strength U depend among other experimental parameters on the lattice potential V_x [31]. The equilibrium properties of the one-dimensional Hubbard model have been intensively studied by a variety of techniques [23, 24, 25, 26], e.g. exact solutions, bosonization, and numerical methods. At low temperature in a system with attractive interaction a superfluid state is formed, whereas for a repulsive interaction the ground state is either a half-filled Mott insulator or, away from half-filling, a Luttinger liquid. However, the non-equilibrium properties are still a challenge. We use the quasi-exact adaptive time-dependent density matrix renormalization group method (adaptive t-DMRG) [27, 28, 29] and perturbative calculations to determine the time-evolution of the system. A periodic modulation of the lattice poten-

tial along the tube $V_x(t) = V_0(1 + \delta V \cos(\omega t))$, where ω is the modulation frequency, can be translated in the lattice description to a periodic modulation of J and U , i.e. $J[V_x(t)]$ and $U[V_x(t)]$. Thus the system is described by an explicitly time-dependent many-body Hamiltonian. In the following J_0 and U_0 will be used for the values $J[V_0]$ and $U[V_0]$.

A system subjected to a periodic modulation of the lattice potential will on average absorb energy if the modulation frequency ω corresponds approximately to the energy ΔE needed to create an excitation, i.e. $\hbar\omega \approx \Delta E$. In the limit of strongly attractive interaction one important class of excitations is the breaking of pairs. In the strongly repulsive limit particle-hole excitations are formed. In both cases these excitations cost an energy of the order of the interaction energy U_0 . Therefore we expect that the application of a periodic lattice modulation can cause energy absorption, if the frequency corresponds to the excitation energy, i.e. $\hbar\omega \approx U_0$. The two cases of attractive and repulsive interaction are related by an electron-hole transformation for one spin species, e.g. $c_{\downarrow,j} \rightarrow (-1)^j c_{\downarrow,j}^\dagger$, which maps $U \rightarrow -U$ [23, 26]. Thus one can restrict the parameters to one sign of the interaction only.

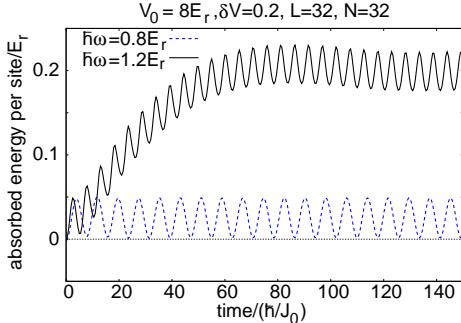


FIG. 1: Absorbed energy $E(t)$ versus time for different modulation frequencies for an initial lattice potential height of V_0 . If the modulation frequency is close to resonance ($\hbar\omega = 1.2E_r$), energy is absorbed, whereas off resonance ($\hbar\omega = 0.8E_r$) no energy absorption takes place.

In Fig. 1 the energy absorption for the case of a periodic modulation, both close to resonance $\hbar\omega \approx U_0$ and off-resonance is shown. In both cases the absorbed energy shows an oscillatory behaviour with the frequency corresponding to the modulation frequency. Off-resonance on average no energy is absorbed by the system, whereas at resonance a clear absorption of energy is visible which saturates at longer times.

The energy absorption versus the modulation frequency is shown in Fig. 2. Here the average value at $t_m = 50\hbar/E_r$ is taken as a measure for the energy absorption [32]. For an initial potential $V_0 = 8E_r$ a clear peak centered around the resonance frequency $\hbar\omega \approx U_0$ is seen (Fig. 2 (a)). For a lower initial potential $V_0 = 4E_r$ (Fig. 2 (b)) we see a broadening of the peak and a clear

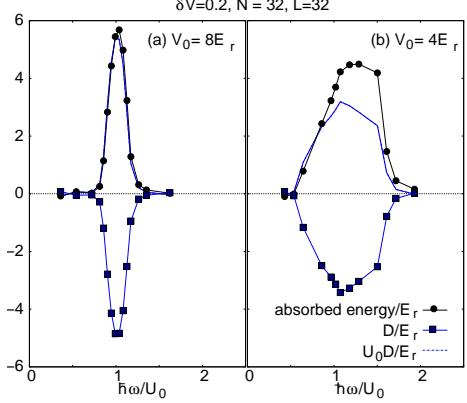


FIG. 2: Energy absorption spectrum (circles) and induced double occupancy D (squares) for (a) an initial lattice potential $V_0 = 8E_r$ and (b) an initial lattice potential $V_0 = 4E_r$, for a strong modulation $\delta V = 0.02$ and $a_s = -9.2\text{nm}$. A clear peak around $\hbar\omega \approx U_0$ arises in both quantities. For a better comparison U_0D is shown as well.

asymmetric form. The maximum of the peak is shifted slightly above the value $\hbar\omega \approx U_0$. These changes are due to the fact that the distance of the ground state energy to the center of the next band is not exactly given by the energy U_0 but shows corrections in J_0 .

In the experiment with bosonic atoms [13] the broadening of the characteristic low momentum peak in the time-of-flight images has been used as a measure for the absorbed energy. In the fermionic experiment the observation of the absorbed energy is more difficult. Due to Pauli's principle for the momentum distribution all momenta up to the Fermi momentum are occupied. Therefore the absorption of energy will only cause a smearing out of the step around the Fermi momentum in time-of-flight images which can not be used to determine quantitatively the amount of energy absorbed [33]. We propose to use the double occupancy in the lattice, i.e. $D = \langle \sum_j n_{j,\uparrow} n_{j,\downarrow} \rangle$ as a quantity which can be observed more easily by projecting pairs of atoms onto molecules [20]. Since for strongly attractive (repulsive) interactions the energy absorption corresponds to a breaking of pairs (generation of particle-hole excitations) we expect that in this limit the energy absorption shows up in the expectation value of the double occupancy. In perturbative calculations we find that up to the quadratic response regime the average induced double occupancy and the average absorbed energy are related simply by a factor U_0 . This result is obtained by expanding $J(t)$ up to first order in δV , neglecting the time-dependence in the interaction, i.e. $U(t) \equiv U_0$, and writing the Hamiltonian as $H(t) = H_0 + g(t)H_K$, where H_0 is the Hubbard Hamiltonian at $t = 0$, H_K is the hopping operator, and $g(t) = (dJ/dV_0)_{\delta V=0}\delta V \cos(\omega t)$. The linear response to this time dependent perturbation gives a purely oscillating contribution to the double occupancy, which averages to zero. Therefore, we consider the quadratic response,

which is given by

$$D_2(t) = \frac{1}{U_0} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dt' dt'' g(t') g(t'') \chi_2(t, t', t'') \quad (2)$$

where $\chi_2(t, t', t'')$ is the quadratic susceptibility. Its relevant term, i.e. the one that gives a non trivial time dependence, can be related to the first order susceptibility,

$$\chi_2^{\text{rel}}(t, t', t'') = -\theta(t' - t'') \frac{d}{dt} \chi_K(t - t') + \text{osc. terms}, \quad (3)$$

where $\theta(t)$ is the step function, and $\chi_K(t) = (1/i\hbar) \langle [H_K(t), H_K(0)] \rangle$. The final expression for the double occupancy is $D_2(t) = D_2(0) - \frac{1}{2}[g(\omega)]^2 \omega t \text{Im} \tilde{\chi}_K(\omega)/U_0 + \text{osc. terms}$, where $\tilde{\chi}_K(\omega)$ is the Fourier transform of $\chi_K(t)$. One finds the same linear growth with time for the expectation value of the total energy, without the factor $1/U_0$. The oscillatory terms, however, are different for both quantities.

In the experimental realization a relatively strong modulation strength δV should be used to get an observable signal. We checked numerically that even for modulation strengths of 20%, the structure of the energy absorption spectrum and the spectrum of the induced double occupancy still contain similar information. In particular we find that the position of the peak agrees for both, whereas deviations occur in the width and amplitude for higher values of the perturbation. Examples for the comparison are shown in Fig. 2.

Since we have seen that the experimentally measurable quantity, the induced double occupancy, can be used as a similar measure as the absorbed energy, we will discuss in the following what kind of information can be extracted from this quantity. Hereby we focus on (i) how to obtain a good measure of the energy necessary to break a pair in the superfluid state or to create a particle-hole excitation in a Mott-insulator or liquid state and (ii) how to gain information about the spin-ordering in a state.

Direct access to the average energy needed to break pairs or to create a particle hole excitations can be obtained from the position of the absorption peak. At zero temperature the dependence of the peak position on the initial interaction strength U_0/J_0 is shown in Fig. 3 for different modulation strengths and fillings (marked by squares and circles). The results were obtained performing the full time-evolution of the system using the adaptive t-DMRG [34]. The position of the peak depends only on the initial interaction strength and not on the size of the perturbation. For strong interactions the dependence is linear. For small values of the interaction strength U_0/J_0 it deviates from the linear form, since the delocalization of the fermions becomes more important and the simple picture of assuming the state to consist of localized particles breaks down [23, 24]. To study the robustness of the peak to the influences of finite temperature we additionally perform a perturbative calculation for small

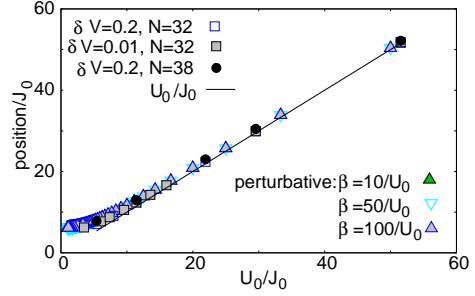


FIG. 3: The position of the peak in the induced double occupancy. Results obtained by a full time-dependent calculation (adaptive t-DMRG) are shown at half filling, $a_s = 9.2\text{nm}$ for a strong perturbation $\delta V = 0.2$ (empty squares), at half filling for a weak perturbation $\delta V = 0.01$ (filled squares), and away of half filling for a strong perturbation $\delta V = 0.2$ (circles). Perturbative results (triangles) are shown for different temperatures $k_B T = 1/\beta$ for small systems sizes ($L = 6$ and $N = 6$). A good agreement between all results is found, which makes the position of the peak a good measure of U_0/J_0 .

system sizes. In Fig. 3 we show the position of the maximum value of the contributions in quadratic response calculations [35]. The collapse of the data for different temperatures shows that the position is mainly independent of temperature. The good agreement between our results shows that the position is a very robust quantity, which is almost independent of temperature, strength of the modulation, size and filling of the system.

In experiments an additional harmonic trapping potential is present. We expect that its main influence on the induced double occupancy is a broadening of the width of the peak, as was found in the bosonic case [19]. In particular, the position of the peak will remain unaffected. In the limit of strong interaction this can be understood by the introduction of potential energy differences between neighbouring sites by the trapping potential. This causes a shift of the excitation energy for the pair breaking or the creation of particle-hole pairs, but with a sign depending on the direction of the excitation. Therefore the position of the peak remains unchanged whereas its form can be broadened. In the experiment with bosonic atoms [13] for strong interaction strength the position of the resonance peak in the energy absorption could be determined approximately up to an accuracy of 20 Hz. Note, that since the broadening of the peak is proportional to J_0 the accuracy is best for strong interaction. In the fermionic case it is hard to estimate the loss of accuracy by the projection onto molecules, but we expect that the accuracy which can be obtained is of the same order of magnitude.

In a two component fermionic system with repulsive interactions the probability to create a particle-hole excitation depends strongly on the spin ordering present in the initial state. In a ferromagnetically ordered state with only a few domain walls particle-hole excitations are strongly suppressed by the Pauli principle, whereas in an

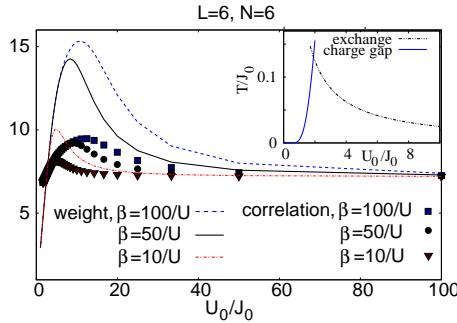


FIG. 4: The weight of the peak in the induced double occupancy for different temperatures $1/\beta$ compared to the nearest neighbour correlations function $4L\langle n_{\uparrow,j}n_{\downarrow,j+1} \rangle$ in a small system with $L = 6$ sites and $N = 6$ particles. The inset shows the competing energy scales influencing the spin ordering.

antiferromagnetically ordered state the creation of particle hole pairs is facilitated. This means that a state which is antiferromagnetically ordered will show more absorption than a paramagnetically or ferromagnetically ordered state. Thus the weight of the absorption peak gives information about the spin ordering. To be more specific, for large U_0/J_0 perturbative calculations yield that the weight is proportional to the nearest neighbour correlation $\langle n_{\uparrow,j}n_{\downarrow,j+1} \rangle$. This can be seen in Fig. 4 where we compare perturbation results for the weight of the absorption and nearest neighbour correlations for different temperatures. At large values of U_0/J_0 we find very good

agreement between the quantities, whereas for smaller interaction the values deviate. A maximum occurs in both quantities at approximately the same finite interaction strength. This is due to two competing processes which destroy the spin order, the delocalization of charge dominating at low U_0/J_0 and the spin exchange dominating at large U_0/J_0 . In the inset in Fig. 4 this competition of the energy scales for the spin ordering, the charge gap and the spin exchange coupling are shown. The maximum in the weight shows the crossover between the two energy scales thus giving information about the spin ordering of the system.

To summarize we have proposed a setup to measure the pair-binding energy, the interaction strength, and the spin-ordering in a Fermi gas in an optical lattice. The proposed experiment observes the double occupancy induced by periodic lattice modulations via the creation of molecules. The robustness of the measurement procedure to external influences such as temperature or a harmonic trapping potential makes an precise experimental determination of the pair-binding energy, the interaction strength – thereby the scattering length – and the spin ordering in the optical lattice possible. Since for strong interactions the proposed measurement is based on a local effect, i.e. the creation of particle-hole pairs, we expect it to hold as well in higher dimensions.

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[31] In our simulation we use parameters corresponding to a gas of K^{40} atoms in the $F = 9/2$, $m_f = -9/2$ and $m_f = -7/2$ states and $\lambda = 826$ nm.
[32] This is determined by smoothening the oscillations in the

- curve by convolution with a Gaussian $\exp(-t^2/(2\Delta T^2))$ with $\Delta T \approx \pi/\omega$.
- [33] A similar smearing is caused by the finite temperature and the trapping potential [30]
- [34] We determine the position a by fitting a Gaussian of the form $c \exp(-(x-a)^2/\sigma^2)$. Note, that the fit by a Gaussian function is not very accurate for small values of U_0/J_0 due to the asymmetric form of the peak.
- [35] We show the position of the maximum value of the δ -peaks, i.e. $1/Z(E_m - E_n)|\langle n|H_K|m\rangle|^2 \exp(-\beta(E_n - E_m)(1 - \exp(-\beta(E_m - E_n))))$. Here E_n are the eigenvalues of the unperturbed Hamiltonian, β gives the inverse temperature.